MILLIMETER-WAVE SPECTROSCOPY OF ETHYLMERCURY HYDRIDE

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The first millimeter-wave rotational spectrum of an organomercury compound, ethylmercury hydride (CH_3CH_2HgH), has been recorded using the Lille fast-scan spectrometer[a] in the frequency range 120 – 180 GHz. The spectroscopic study is complemented by quantum chemical calculations taking into account relativistic effects on the mercury atom. The very good agreement between theoretical and experimental molecular parameters validates the chosen ab initio method, in particular its capability to predict the accurate values of the quartic centrifugal distortion constants related to this type of compound. Estimations of the nuclear quadrupole coupling constants are not as predictive as the structural parameters but good enough to satisfy the spectroscopic needs. In addition, the orientation of the H–Hg–C bonds axis deduced from the experimental nuclear quadrupole coupling constants compares well with the corresponding ab initio value. From the good agreement between experimental and theoretical results, together with the observation of the six most abundant isotopes of mercury, ethylmercury hydride is unambiguously identified and its calculated equilibrium geometry is confirmed.

[a] Alekseev, E.A. et al. *Radio Physics and Radio Astronomy* **3** (2012) 78.